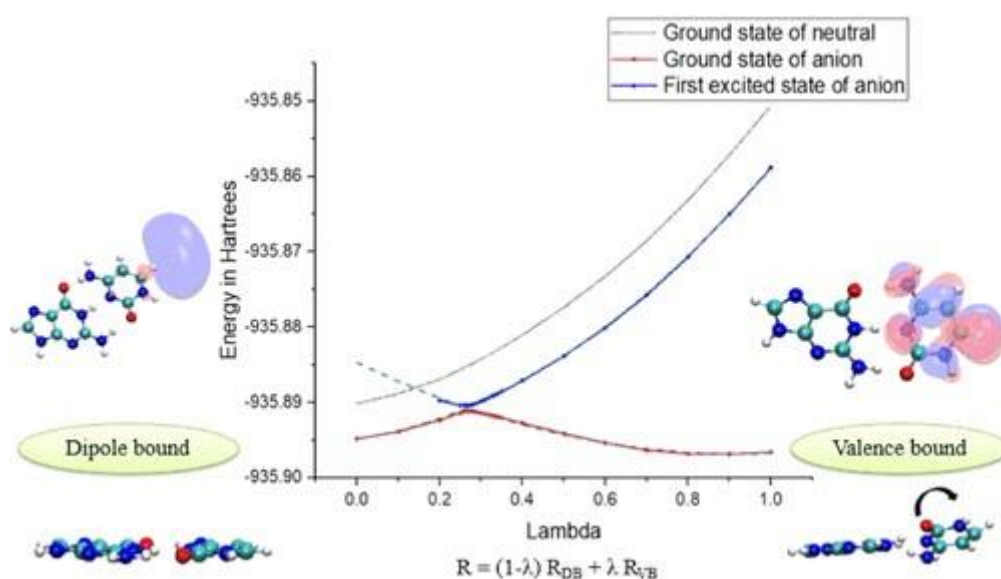


The Electron Attachment Induced Radiation Damage to Genetic Materials: The Role of Water

Achintya Kumar Dutta

Indian Institute of Technology Bombay, Powai, Mumbai 400076

Radiation damage to genetic material is one of the active fields of chemical research with implications in both the cause and cure of cancer. The origin of the damage for a long time is attributed to the ionization and excitation process created by the high energy radiation. But recent experiments have highlighted the critical role played by the low-energy secondary electron in the radiation damage process[1]. Water has been shown to accelerate the process of radiation damage. We have shown that the initial electron attached state is localized on the water, and the water bound state act as a doorway[2] for the electron attachment to nucleobases. Subsequently, the electron gets transferred to the nucleobase due to the mixing of the electronic and the nuclear degrees of freedom. The newly developed EOM-CCSD based QMMM simulations[3] show that the rate of electron transfer increases in the presence of bulk water, and takes place in the ultrafast time scale. The local structure of water around the nucleobase anion plays a crucial role in the electron attachment process. The computed adiabatic electron affinity and the electron transfer rate show good agreement with the experimental results, validating our proposed mechanism[4].



References:

- [1] J. Ma, F. Wang, S. A. Denisov, A. Adhikary, M. Mostafavi, *Sci. Adv.*, **2017**, 3.12, e1701669.
- [2] D. Tripathi and A.K. Dutta, *J. Phys. Chem. A* **2019**, 123, 46, 10131-10138.
- [3] S. Haldar, C. Riplinger, B. Demoulin, F. Neese, F., R. Izsak, and A. K. Dutta. *J. Chem. Theory. Comput.* **2019**, 15, 2265-2277
- [4] M. Mukherjee, D. Tripathi, and A. K. Dutta. (arXiv:1911.00335) **2019**.